Mechanical molecular models and haptic reasoning

By: Mathieu Charbonneau

Up to the 1960s, biochemistry and molecular biology were profoundly influenced by the deployment and diversity of a peculiar kind of research tool: mechanical molecular models (Francoeur, 1997, 2000). Although such physical models of molecular structures have been replaced by simulated or virtual models in modeling tasks (Francoeur & Segal, 2004), the building of scale models of molecular structures from tangible components was once an important part of the practice of biologically oriented chemists. This model-building strategy directly served the scientist's research interests. The construction and manipulation of plastic, wooden and metallic models of possible molecular structures played a central part in an informed trial-anderror research strategy that proved especially useful in elucidating complex molecular structures such as those of organic macromolecules. In the late 1940s and early 1950s, chemist and biochemist Linus Pauling pioneered the systematic use of these "tinker toys" for the structural determination of compounds (e.g. Corey & Pauling, 1953), a research strategy historian of science Lily Kay has characterized as a "molecular architecture epistemology" (Kay, 1993, p. 262). This pervasive research strategy led to new scientific knowledge, including major breakthroughs, by stimulating the scientist's imagination and pointing to new research avenues (Laszlo, 1993, 2000). Certainly the most famous example of such successful use of molecular models is James Watson's and Francis Crick's use of this research strategy in discovering the basic structure of the DNA molecule. The metallic model they used was not simply a dramatic display in an extravagant showcase: it was itself a tool for research and served as a locus for discovery. And this case is no anomaly—the use of such models for complex structural determination was typical rather than exceptional (Francoeur, 1997).

Although nowadays these tangible models are seldom encountered outside undergraduate biochemistry courses, their historical importance as research tools guarantees their place in the standard iconography of science, making them familiar even to the layman. The role these physical models have played in scientific discovery has received little attention, with most scholarly focus being aimed to their supporting roles as pedagogical devices manipulated for better learning/memorization of a selected molecule's structure or used as visual support in classrooms (e.g. Coll, 2006). Though the historian Robert Olby (1974) does mention here and there the use of such models, and describes in detail Pauling's paper-made alpha-helix model (Olby, 1974, p. 208-201), there is no systematic discussion of the importance and role these physical models played—even though they did play a central role in paving the way for contemporary molecular biology. Philosophers have paid even less attention to these models but, when attended, the discussion centers on the more general aspects of representing and modeling (e.g. Giere, 2012), such as the scientists' struggle with visualizing three-dimensionality by a two dimensional media (e.g. Francoeur, 1997; de Chadarevian & Hopwood, 2004; Gooding, 2006)). More generally, in the SEP entry on Models in Science, Frigg and Hartmann write about physical models that they "[…] do not give rise to any ontological difficulties over and above the well-known quibbles in connection with objects, which metaphysicians deal with." (Frigg and Hartmann, 2012, section 2.1). From this latter perspective, there seems to be little more to physical models of molecular structures than a means to represent more accessibly the three-dimensional structure of a given molecule.

The trouble with this view is that it does not account for the actual practice of using physical models as research tools nor for the manner by which new scientific knowledge is produced when doing so. When a modeler aims to solve a molecule's structure with the aid of such physical models, she explores different combinations of model parts, makes measurements, often disassembling and reassembling the models built. These interactive manipulations exploit the mechanical properties of the models, properties which are not reducible to matters of visualization. Moreover, the use of these physical models has often replaced the deployment of mathematical calculations in molecular modeling contexts. This introduces a pragmatic dimension that cannot be ignored: when compared with geometrical drawings and mathematical calculations, physical models appear to be costly (in time, energy and money) and cumbersome replacements for clean paper work. I will argue here that mechanical molecular models are not just static representations, equivalent to flat geometrical and mathematical calculations with a three-dimensional twist; they have something more that makes them non-trivially different from their inscriptional counterparts.

The main claim of this paper is that mechanical molecular models (henceforth, 'M-models') were used as research tools that, through their mechanical properties, augment and extend the modeler's cognitive capacities and performances. . Instead of relying on mathematical tools or solely on internal cognitive capacities, the architect manipulates these material props in such a way as to become more efficient in her problem solving. This is done by replacing extensive mathematical calculations by a different set of cognitive capacities such as visuospatial and haptic reasoning. Moreover, exploitation of the materiality of the M-model by informed manipulations on the part of the architect allows the Mmodel to take an active part in the cognitive work required to solve a complex molecule's structure. Mmodels thus facilitate and extend the architects performances by integrating the inherent causality of the M-models materiality to serve as part of the cognitive process required to solve molecular modeling tasks.

Moreover, I will argue that their component parts were designed, built and used to serve such cognitive functions. By an intelligent use of M-Models' material properties, the molecular architect's manipulations of the model parts enhanced her cognitive performances by facilitating the modeling task. This shows that, contrary to Frigg and Hartmann's summary, there is more to the ontology of physical models than what has been led to believe by current philosophical investigations. Recasting Mmodels as cognitive augmentations opens the way for a new horizon of research in the philosophy of science about the scientific uses of physical models.